Spin-Orbital Entanglement and Phase Diagram of Spin-orbital Chain with $SU(2) \times SU(2)$ Symmetry

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Spin-orbital entanglement in quantum spin-orbital systems is quantified by a reduced von Neumann entropy, and is calculated for the ground state of a coupled spin-orbital chain with $SU(2) \times SU(2)$ symmetry. By analyzing the discontinuity and local extreme of the reduced entropy as functions of the model parameters, we deduce a rich phase diagram to describe the quantum phase transitions in the model. Our approach provides an efficient and powerful method to identify phase boundaries in a system with complex correlation between multiply degrees of freedom.

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Exotic states associated with the orbital degrees of freedom in transition-metal oxides have attracted considerable interest recently. Examples of such systems with spin-orbital couplings include spin-gap materials $Na_2Ti_2Sb_2O$ and NaV_2O_5, manganites $La_{1-x}Sr_xMnO_3$, and V_2O_3 [1, 2, 3, 4, 5]. Intriguing physical properties in these systems include the emergence of orbital ordering, the appearance of complex coupled excitations involving both spin and orbital degrees of freedom. Starting from a multi-band Hubbard model at strong coupling limit and at the integer fillings of electrons per unit cell, the charge degree of freedom is frozen and one may derive an effective spin-orbital model [6, 7]. One of the simplest such systems is the $SU(2) \times SU(2)$ model with $SU(2)$ symmetries for spin-1/2 operator $\mathbf{S}_i$ as well as for pseudospin-1/2 operator $\mathbf{T}_i$ representing two degenerate orbitals. There have been a lot of activities recently on the one-dimensional spin-orbital coupled systems [8, 9], especially on its phase diagram [10, 11, 12, 13, 14]. Rich quantum phases include both conventional ferromagnetic/antiferromagnetic gapless phases and symmetry broken gapped states. In the strong coupling regime where the interplay between spin and orbital quantum fluctuations is crucial, the detailed phase diagram still remains controversial and a more comprehensive understanding is awaited.

More recently, the investigation of quantum entanglement from the perspective of quantum information theory has gained much insight for a deeper understanding of quantum many particle physics, especially quantum phase transitions. Many theoretical studies have been devoted to the entanglement in one dimensional spin-1/2 systems [15, 16, 17, 18, 19, 20] and in interacting fermion and boson systems [21, 22]. Quantum entanglement has been quantified in terms of the spin-spin concurrence [15], contiguous block entanglement [18], and sublattice entanglement [20, 22]. There are evidences to suggest a close connection between quantum phase transition and local extreme or singularity of the quantum entanglement when it is measured appropriately [20]. In the coupled spin-orbital systems, one expects the spin-orbital entanglement (SOE) to be important. In particular, near a quantum transition point, one may naturally expect that the entanglement may manifest itself accordingly. Recent theoretical study has also demonstrated that the SOE could lead to the violation of the Goodenough-Kanamori rules [23].

In this paper, we propose a reduced von Neumann entropy to quantify the SOE, which measures the interplay between spin and orbital degrees of freedom of the quantum states. We use small size exact numerical method to calculate the reduced entropy of the ground state of the spin-orbital chain given by Hamiltonian Eq. (1) and study its relation with the quantum phase transition of the system. Our results show that this novel measure of the entanglement can reveal faithfully the quantum transition points and phase boundaries of the complex phase diagram of the system. Our results indicate that the strategy of evaluating entanglement measure is powerful and efficient for extracting valuable information of the quantum systems.

We consider a one-dimensional spin-orbital Hamiltonian with $SU(2) \times SU(2)$ symmetry,

$$H = \sum_i \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} + x\right)\left(\mathbf{T}_i \cdot \mathbf{T}_{i+1} + y\right), \qquad (1)$$

where $\mathbf{S}_i$ are spin-1/2 operators while $\mathbf{T}_i$ denote the orbital pseudo-spin 1/2 operators. x and y are two tuning parameters. At $x = y$, the model has an interchange symmetry between spin and orbital. The model at $x = y = 1/4$ is a special case possessing a higher $SU(4)$ symmetry, and there are three gapless modes (spin, orbital and spin-orbital) in the low-lying excitations [24, 26]. It is also known that the model at $x = y = 3/4$ has an exact ground state, in which the spin and orbital form dimerized singlets in a staggered pattern, and the doubly degenerate ground states can be expressed as gapped matrix product state [27].

In the spin-orbital model, the importance of the SOE has long been recognized [23, 24]. However, a quanti-

tative measure for the entanglement is still lacking. We propose to measure the SOE by a reduced von Neumann entropy defined as

$$S^{so} := -\mathrm{tr_s}\left(\rho_\mathrm{s}\log_2\rho_\mathrm{s}\right), \tag{2}$$

where $\rho_s \equiv \mathrm{tr_o}|\Psi\rangle\langle\Psi|$ is the reduced density matrix of the spin part in the state $|\Psi\rangle$ by integrating out all the orbital degree of freedom. Obviously, Eq. (2) gives $S^{so}=0$ if spin **S** and orbital **T** are decoupled. The motivation for such a measure is to better reveal the correlation between two distinctive degrees of freedom. This measure is similar to the recent proposal of the reduced entropy S_L of a block of subsystem in study of the relations between entanglement and quantum phase transition, where S_L is defined by

$$S_L := -\mathrm{tr}\left(\rho_\mathrm{L}\log_2\rho_\mathrm{L}\right), \tag{3}$$

where $\rho_L \equiv \mathrm{tr_L}|\Psi\rangle\langle\Psi|$ is the reduced density matrix for a block of subsystem B_L. The analogy of the SOE with the block subsystem becomes more clear if we map the model of Eq. (1) onto a two-leg "spin" ladder system with one chain described by spin **S** and the other chain by orbital **T** and the two sites on each leg are coupled by a four-operator interactions [28].

Let us first examine the SOE defined in Eq. (2) in a few simplest cases. For a single site system, the SOE has a one-to-one correspondence to the two pure spin-1/2 system with one spin for **S** and the other for **T**. For a two-site system, the spin (orbital) states can be either a singlet $|\Psi^s_S\rangle$ ($|\Psi^s_O\rangle$) or triplet $|\Psi^t_S\rangle$ ($|\Psi^t_O\rangle$). It is easy to check that $S^{so}=0$ for all the spin-orbital decoupled states, and $S^{so}=1$ for the state $1/\sqrt{2}(|\Psi^s_S\rangle|\Psi^t_O\rangle \pm |\Psi^t_S\rangle|\Psi^s_O\rangle)$. Next we proceed to the 4-site (1234) cluster, which is the smallest system size to have $SU(4)$ singlet state $|SGL\rangle$. This $|SGL\rangle$ state contains 24 terms, and is rotational invariant under the fifteen $SU(4)$ generators [24, 25, 29]. After tracing over the orbital degrees of freedom, we find $S^{so}=1$ for this high symmetry state. For the dimerized state at $(x=y=3/4)$, it is known that its ground state is a matrix product state in both spin and orbital part [27]. After some algebra, we find its value of entanglement is about 0.40.

In what follows we will calculate the ground state SOE of the Hamiltonian (1) in a finite size system. We will demonstrate the close connection between SOE and the quantum phase transitions in the model. Since the Hamiltonian has a rotational symmetry around the z-axes in **S**-space as well as in **T**-space, the exact diagonalization calculations are carried out in an invariant subspace with $S_z=0$ and $T_z=0$ to get the ground state $|\Psi_G\rangle$, from which we construct the density matrix for the whole system. The reduced density matrix ρ_L of spin part is obtained by tracing out the orbital degree of freedom, and compute its reduced entropy. In our calculation, the chain length ranges from 8 to 12.

The spatial profiles of SOE S^{so}/L as a function of x and y are displayed in Fig. 1. A salient feature shows

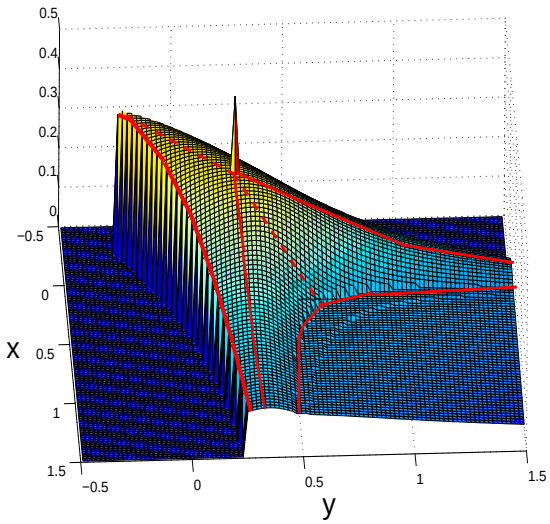

FIG. 1: The rescaled SOE S^{so}/L ($L=8$) as a function of the x and y. The phase boundaries (red lines) are drawn to guide the eyes.

the existence of zero entanglement regime. When either $\mathbf{S}_i$ or $\mathbf{T}_i$ are aligned ferromagnetically, this model has no frustration and qualitative results can be obtained from physical considerations alone. Intuitively, for $x>-1/4$ $(x<-1/4)$ and $y<-1/4$ $(y>-1/4)$, the ground states are antiferromagnetic for spin **S** and ferromagnetic for orbital **T** (and vice versa). In the case of large negative x and y, the ground state is the ferromagnetic state with respect to both **S** and **T**. These three conventional states correspond to the decoupling between the spin and orbital degrees of freedom. Therefore, these states have zero SOE. On the other hand, if both **S** and **T** are coupled antiferromagnetically, the four-operator term may frustrate the system, which may lead to the emergence of various non-trivial ground states with finite values of SOE. As depicted in Fig. 1, there are boundary lines with finite discontinuous jump of SOE between the zero-value and finite-value regions which indicates a first-order phase transition. Ground states of the boundary lines of the fully ferromagnetic spin and orbital phases are highly degenerate. It is obvious that the quantum fluctuation effect pushes the classical phase boundary closer to the symmetric line $x=y$.

Two special points manifest themselves clearly: the $SU(4)$ symmetric point corresponds a local maximum of S^{so}/L while the dimerized state point corresponds a local minimum. This feature may be simply understood as follows. At the $SU(4)$ point, there is the largest correlation between spin and orbital degrees of freedom, while at the dimer phase point, both the spin **S** and orbital **T** are weakly coupled so that the entanglement is much suppressed. In addition, the symmetric line $x=y$ is more special and interesting. In Fig. 1, along the line (referred to as the line A) connecting the point $(-1/4,-1/4)$ and the $SU(4)$ point where both of them have high symme-

tries, S^{so}/L reaches the local maxima (ridge-like), while along the line (referred to as the line B) connecting the $SU(4)$ point and (0.66,0.66), it behaves as the local minima (valley-like). According to our previous analysis and wisdom [20, 22], we know that both the ridges and valleys may correspond to phase boundaries. We conclude here that both lines A and B may serve as phase boundaries. It is worth noting that the $SU(4)$ symmetric point is a multi-critical point. There are four distinct neighboring quantum phases around this point. For example, moving off this symmetric point, one may enter the gapped states to the right upwards or enter the gapless phases to the left downwards. These results are likely supported by other studies. (i) The critical line A is consistent with that of the analysis by Yamashita *et al.* [12]. (ii) In a recent Schwinger boson mean field study [30], both spin and orbital valence bond states are found in the parameter region separated by the critical line B. Around the dimerized state point, one may observe that there exists a curved phase boundary line dividing the regions where the discontinuity of first derivative of entanglement as a function of parameters occurs. The high temperature series expansion approach suggests the existence of two distinct gapped phases in the parameter region for both positive x and y [14]. Our calculation supports the existence of such gapped phases.

For the large x and y region, mean field studies always suggest that the ground state is the antiferromagnetic state with respect to **S** and **T**. In that case, we would expect that its corresponding SOE is equal to zero. However, the SOE in this parameter region shows plateau-like behavior with finite value, which contradicts the conclusion of mean field studies. Since the well-known dimerized state point is located within the large x and y region, we conclude that this phase regime belongs to the gapped dimerized state rather than the gapless antiferromagnetic phase. It is worth noting that the strength of SOE may be regarded as an indicator to discern how good the mean field approximation will be. In the strongly coupled regime, the interplay between spin and orbital quantum fluctuations may be important and leads to some highly nontrivial quantum phases. Therefore it is necessary to consider the effects of quantum fluctuations more seriously beyond the mean field theory. Certainly, we also find that both entanglement measures vanish in the infinitely large limits of x and y.

To study the additional entanglement between the intercalated sublattices of composite degrees of freedom and to best reveal all possible quantum phase boundaries, we also look into the standard sublattice entanglement [20, 22], which is obtained by tracing out both spin and orbital degrees of freedom at even (or odd) sites in the present chain. In Fig. 2, we plot the sublattice entanglement versus the coupling parameters. It is interesting to note that there is roughly one-to-one correspondence of local extreme and discontinuity between these two measures of entanglement. In contrast to that of SOE, the $SU(4)$ point reaches a local minimum of sublattice entanglement while the dimerized state point corresponds to a local maximum. Since the SOE mainly captures the correlation between the spin and orbital degrees of freedom while the sublattice entanglement focuses on the correlation between the intercalated sublattices of composite degrees of freedom, these two measures may provide certain complementary information. In the case of conventional ferromagnetic/antiferromagnetic phases, the SOE vanishes while the sublattice entanglement remains nonzero. Thus the measure of SOE is unlikely to distinguish these conventional phases. Instead, in Fig. 2, these phases are clearly separated. In addition, the enhancement of sublattice entanglement for the gapped dimerized state is clearly observed.

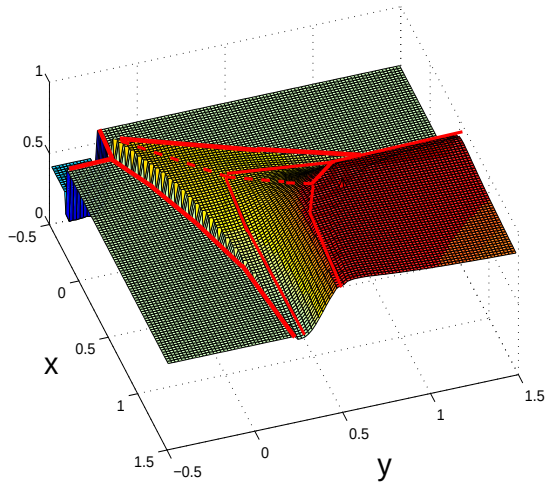

FIG. 2: The rescaled sublattice entanglement $S_{L/2}/L$ ($L = 8$) as a function of the x and y. The phase boundaries (red lines) are essentially the same as that of Fig. 1.

Quantum phase diagram can be distilled from the analysis of the spatial profiles of entanglement as a function of parameters. In other words, both the ridges and valleys in the three-dimensional plot may correspond to possible phase boundaries. Derived from the numerical results presented in Figs. 1 and 2, we plot the phase boundaries of a coupled spin-orbital chain for $L = 8$ in Fig. 3. The results for $L = 12$ are essentially the same. There are totally eight distinct quantum phases. Most phase boundaries are in good agreement with previous studies [10, 12, 13, 14]. Phases I, II and III, are conventional spin and orbital ferromagnetic or antiferromagnetic states. Phase IV and V belong to gapless states. [12]. Phase VI and VII may correspond to orbital and spin valence bond phases [30], respectively. In view of the fact that the exact ground state at the point $(3/4, 3/4)$ belongs to staggered dimerized singlet and this dimerized state point is located within phase VIII, we conclude that the phase VIII is a staggered dimerized singlet state. It is remarkable that the most comprehensive phase diagram is now efficiently and straightforwardly

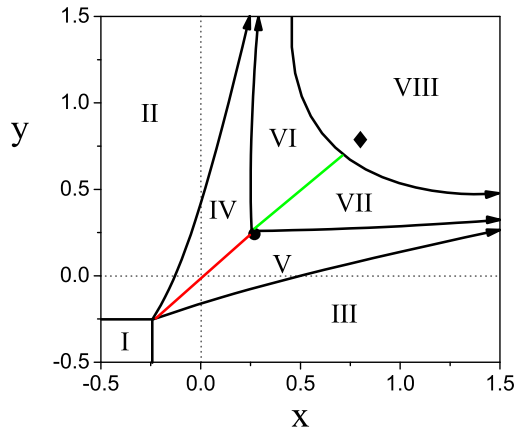

FIG. 3: Ground state phase diagram of a coupled spin-orbital chain. The dotted point is at (1/4,1/4) while the diamond point is located at (3/4,3/4). Eight distinct phases are identified according to the analysis of entanglement as a function of parameters x and y. See text for details.

obtained.

Since the coupled spin-orbital chain can be regarded equivalently to a two-leg spin ladder with four-spin interactions, we may also employ the measure of concurrence to quantify the bipartite entanglement in terms of spin-spin, orbital-orbital as well as spin-orbital concurrence. Our results show that the concurrence can merely show a few features of phase diagram such as the conventional phases I, II and III, but unfortunately, it fails to identify the detailed phase diagram in the strong coupling regime. Another scenario is to analyze so-called single-site entanglement. In this case, we obtain the reduced density matrix by tracing out all degrees of freedom except for a single site and then get its reduced entropy. However, we are still unable to identify many phase boundaries. In our opinion, the failure of these two measures highlights the importance of the nonlocal many body correlation effect in characterizing some nontrivial quantum phases.

In conclusion, we present a novel approach to study phase diagram of the coupled spin-orbital chain by coherently examining the entanglement related to two distinctive degrees of freedom. The analysis of the SOE supplemented by the sublattice entanglement scenario enables us to establish an one-to-one link between its local extreme/discontinuity and quantum transition points. The most comprehensive phase diagram has been deduced for the first time based on exact numerical results for a finite lattice system. Our approach presents a superior and efficient way to identify quantum phase transitions in a coupled spin-orbital system. The present work may shed new light on the understanding of the complicated interplay among charge, spin and orbital degrees of freedom in transition-metal oxides in terms of entanglement.

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where $(12)_{S(O)}$ stands for the spin (orbital) singlet state of the sites 1 and 2.
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